

Log

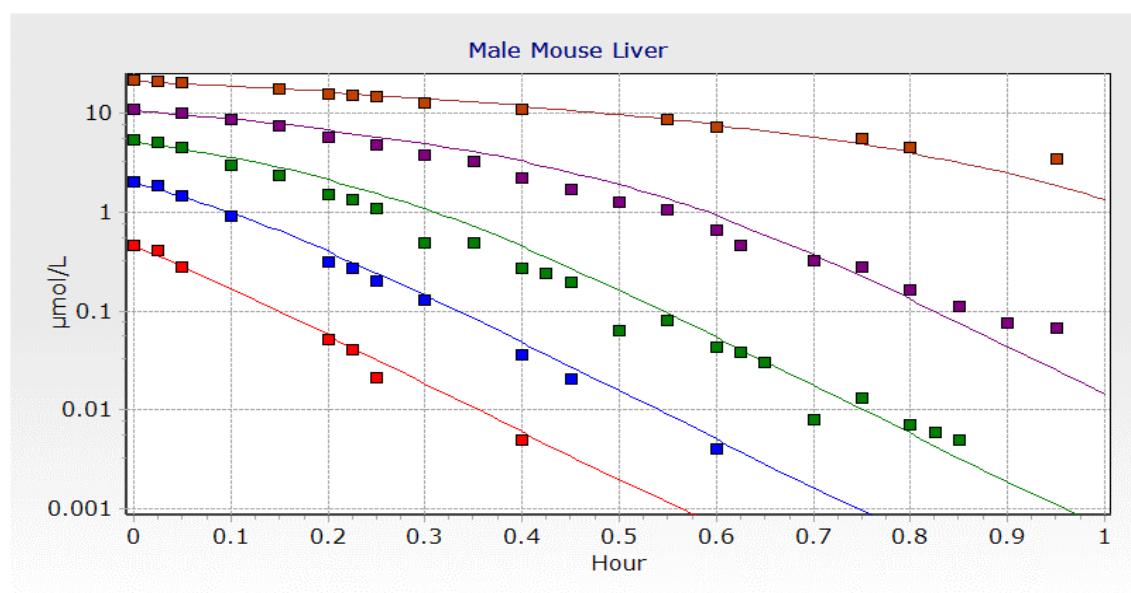
Male

		Average	95% CI
Vmax	$\mu\text{mol}/\text{hr}/\text{mg protein}$	-1.38	-1.43 -1.33
Km	$\mu\text{g}/\text{L}$		
Kg	L/hr	-0.80	-1.07 -0.42

EXP

Male

		Average	95% CI
Vmax	$\mu\text{mol}/\text{hr}/\text{mg protein}$	0.25	0.24 0.26
Km	$\mu\text{mol}/\text{L}$	1.000	
Kg	L/hr	0.45	0.34 0.65



Male

```
gelman.dia autoburnin=FALSE)
Potential scale reduction factors:
```

	Point	est.	Upper	C.I.
LI		1	1	
Vmax		1	1	
Kgi		1	1	

Multivariat psrf

```
1
>
> summary(x1)

Iterations = 1:14000
Thinning interval = 1
Number of chains = 1
Sample size per chain = 14000

1 Empirical mean and standard deviation plus standard error of the

Mean SD Naive SE Time-series
LI 0.3231 0.02717 0.00023 0.000375
Vmax -1.3802 0.02339 0.000198 0.000904
Kgi -0.7968 0.16306 0.001378 0.006451
```

2 Quantiles for each variable:

```
2.50% 25% 50% 75% 97.50%
LI 0.2747 0.304 0.321 0.3408 0.3809
Vmax -1.4273 -1.396 -1.3799 -1.3641 -1.3348
Kgi -1.0732 -0.905 -0.8133 -0.7069 -0.4233
```

```
> summary(x2)

Iterations = 1:14000
Thinning interval = 1
Number of chains = 1
Sample size per chain = 14000

1 Empirical mean and standard deviation plus standard error of the

Mean SD Naive SE Time-series
LI 0.3238 0.02802 0.000237 0.000387
```

Vmax	-1.381	0.02402	0.000203	0.001018
Kgi	-0.7916	0.16736	0.001414	0.006983

2 Quantiles for each variable:

	2.50%	25%	50%	75%	97.50%
LI	0.2744	0.3041	0.3216	0.341	0.3846
Vmax	-1.4281	-1.3974	-1.381	-1.3641	-1.3353
Kgi	-1.0709	-0.9095	-0.8075	-0.6919	-0.4267

> summary(x3)

Iterations = 1:14000
 Thinning interval = 1
 Number of chains = 1
 Sample size per chain = 14000

1 Empirical mean and standard deviation plus standard error of the

	Mean	SD	Naive	SE	Time-series
LI	0.3232	0.028	0.000237	0.000403	
Vmax	-1.3818	0.02295	0.000194	0.000859	
Kgi	-0.7879	0.15996	0.001352	0.006047	

2 Quantiles for each variable:

	2.50%	25%	50%	75%	97.50%
LI	0.2748	0.3031	0.3215	0.3409	0.3836
Vmax	-1.4275	-1.3969	-1.3823	-1.3658	-1.3369
Kgi	-1.0623	-0.8962	-0.8005	-0.6956	-0.4271

for each variable,
mean:

SE

for each variable,
mean:

SE

for each variable,
mean:

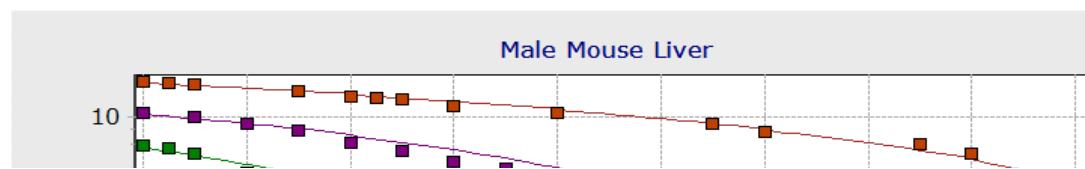
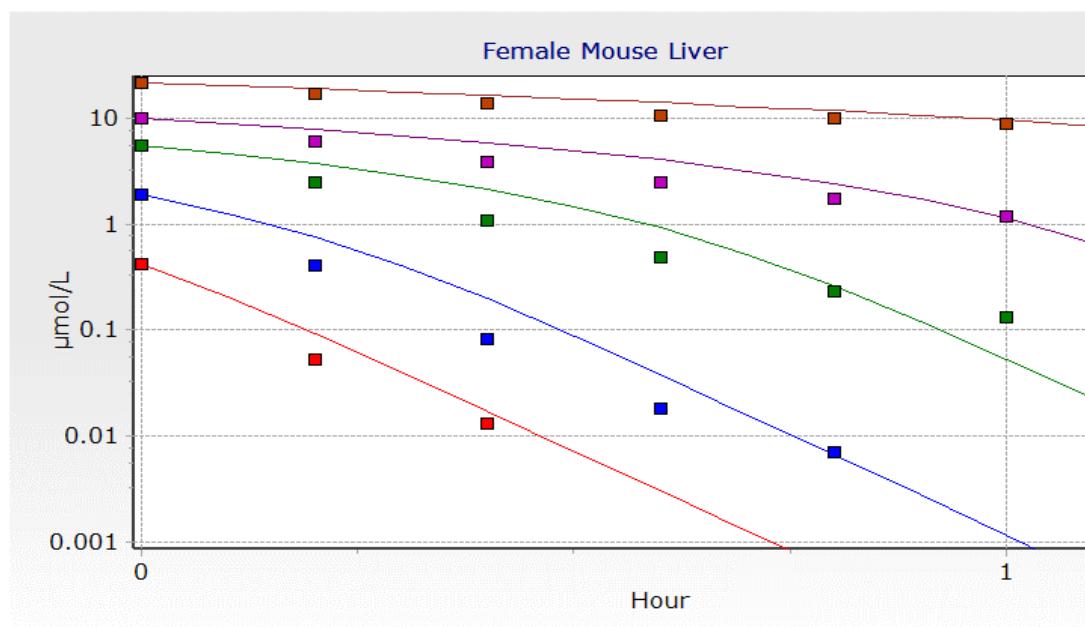
SE

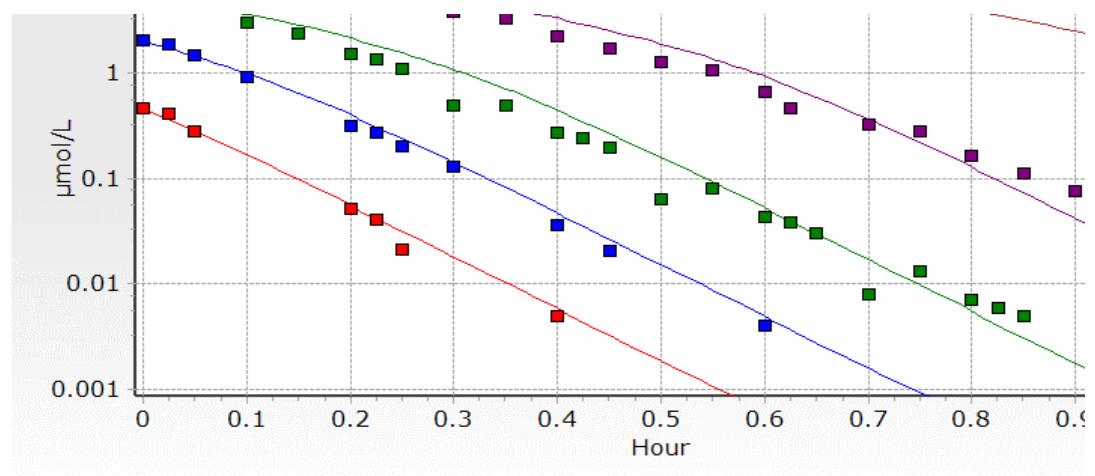
		Female		
Log	Vmax	Average	95% CI	
		μmol/hr/mg protein	-2.18	-2.37
	Km	μg/L	-0.47	-0.81

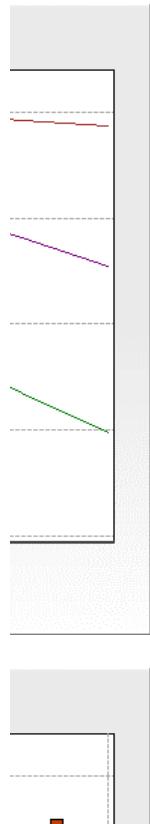
		Male		
EXP	Vmax	Average	95% CI	
		μmol/hr/mg protein	-1.39	-1.45
	Km	μg/L	-0.01	-0.12

		Female		
EXP	Vmax	Average	95% CI	
		μmol/hr/mg protein	0.11	0.093
	Km	μg/L	0.63	0.44

		Male		
EXP	Vmax	Average	95% CI	
		μmol/hr/mg protein	0.25	0.24
	Km	μmol/L	0.99	0.89







Female

```
gelman.dia autoburnin=FALSE)
Potential scale reduction
```

	Point est.	
LI	1	1
Vmax	1.01	1.02
Km	1.01	1.02

Multivariat psrf

1.01

```
>
> summary(x1)
```

```
Iterations = 6.291667
Thinning interval = 
Number of chains
Sample size per
```

1 Empirical mean
plus standard

	Mean	SD
LI	0.4655	0.07326
Vmax	-2.1787	0.09833
Km	-0.4672	0.17677

2 Quantiles for

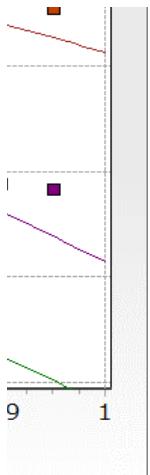
	2.50%	25%
LI	0.3491	0.4136
Vmax	-2.3712	-2.2454
Km	-0.8137	-0.5836

```
> summary(x2)
```

```
Iterations = 6.291667
Thinning interval = 
Number of chains
Sample size per
```

1 Empirical mean
plus standard

	Mean	SD
LI	0.465	0.07277



Vmax	-2.1639	0.10166
Km	-0.4396	0.18183

2 Quantiles for

	2.50%	25%
LI	0.3463	0.4127
Vmax	-2.3616	-2.2324
Km	-0.7926	-0.5588

> summary(x3)

Iterations	=	6.291667
Thinning interval	=	
Number of chains	=	
Sample size	=	per

1 Empirical mean
plus standard

	Mean	SD
LI	0.4673	0.07419
Vmax	-2.1619	0.09912
Km	-0.4351	0.17966

2 Quantiles for

	2.50%	25%
LI	0.3502	0.4161
Vmax	-2.3616	-2.2276
Km	-0.8013	-0.5517

Male

gelman.dia

Potential

factors:

Upper	C.I.	LI
		Vmax
		Km

Multivariat

	1.02
>	
>	

Iterations

1

Thinning

= 1

Number

chain = 9000 Sample

Sample

and standard deviation for each variable, 1

error of the mean:

Naive SE Time-series SE

0.000772	0.001363	LI
0.001037	0.006938	Vmax
0.001863	0.011667	Km

each variable: 2

50%	75%	97.50%	
0.4545	0.509	0.6322	LI
-2.1829	-2.114	-1.9756	Vmax
-0.4733	-0.353	-0.1034	Km

>

Iterations

1

Thinning

= 1

Number

chain = 9000 Sample

Sample

and standard deviation for each variable, 1

error of the mean:

Naive SE Time-series SE

0.000767	0.001428	LI
----------	----------	----

0.001072	0.006972	Vmax	
0.001917	0.012235	Km	
each variable:		2	
50%	75%	97.50%	
0.4574	0.5077	0.63163	LI
-2.1643	-2.0982	-1.96113	Vmax
-0.4383	-0.3194	-0.07958	Km
>			
1			Iterations
=	1		Thinning
chain	=	9000	Number
Sample			
and standard deviation for each variable,		1	
error of the mean:			
Naive SE	Time-series SE		
0.000782	0.001699	LI	
0.001045	0.006426	Vmax	
0.001894	0.011763	Km	
each variable:		2	
50%	75%	97.50%	
0.457	0.5078	0.6369	LI
-2.1606	-2.0973	-1.964	Vmax
-0.4349	-0.3144	-0.0897	Km

```
autoburnin=FALSE)
scale      reduction factors:
```

Point	est.	Upper	C.I.
1	1		
1.02	1.07		
1.02	1.07		

```
psrf
```

```
summary(x1)
```

```
=          6.291667
interval =          1
of        chains =          1
size     per     chain =         9000
```

```
Empirical mean and standard deviation for each variable,
plus standard error of the mean:
```

Mean	SD	Naive	SE	Time-series SE
0.32214	0.0267	0.000281	0.000637	
-1.38777	0.02885	0.000304	0.002532	
-0.01135	0.05151	0.000543	0.004512	

```
Quantiles for each variable:
```

2.50%	25%	50%	75%	97.50%
0.2753	0.30395	0.320739	0.33858	0.37931
-1.4477	-1.4061	-1.38576	-1.36762	-1.33445
-0.1216	-0.04315	-0.00819	0.02475	0.08457

```
summary(x2)
```

```
=          6.291667
interval =          1
of        chains =          1
size     per     chain =         9000
```

```
Empirical mean and standard deviation for each variable,
plus standard error of the mean:
```

Mean	SD	Naive	SE	Time-series SE
0.323134	0.02793	0.000294	0.00067	

```
-1.38562  0.03513  0.00037  0.003517  
-0.00794  0.06247  0.000659  0.006198
```

Quantiles for each variable:

	2.50%	25%	50%	75%	97.50%
0.2759	0.30348	0.321391	0.34027	0.3818	
-1.4509	-1.40968	-1.38587	-1.36035	-1.3192	
-0.1258	-0.05013	-0.00971	0.03511	0.1199	

summary(x3)

```
=          6.291667  
interval =          1  
of        chains =          1  
size      per     chain =          9000
```

Empirical mean and standard deviation for each variable,
plus standard error of the mean:

Mean	SD	Naive	SE	Time-series SE
0.3241	0.02736	0.000288	0.000623	
-1.3956	0.03277	0.000345	0.003328	
-0.0256	0.05851	0.000617	0.006113	

Quantiles for each variable:

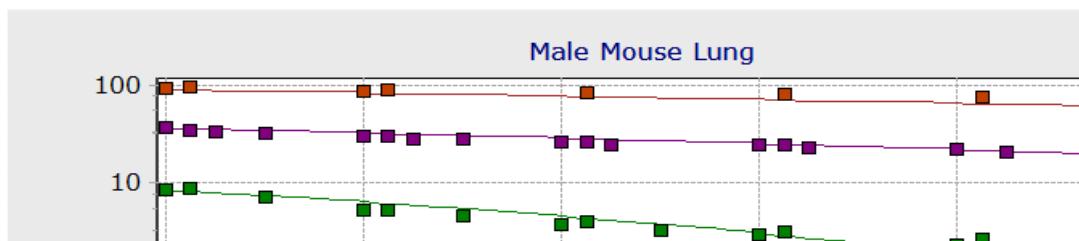
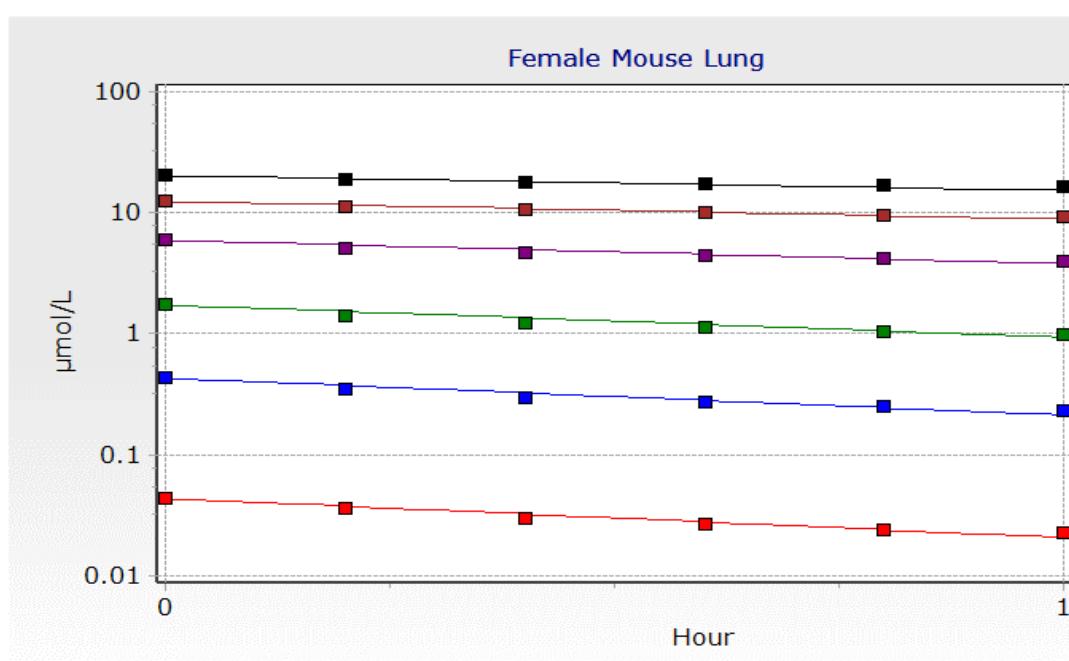
	2.50%	25%	50%	75%	97.50%
0.2746	0.30512	0.3225	0.34162	0.38261	
-1.4586	-1.41795	-1.3959	-1.37222	-1.33255	
-0.1418	-0.06374	-0.0271	0.01564	0.08555	

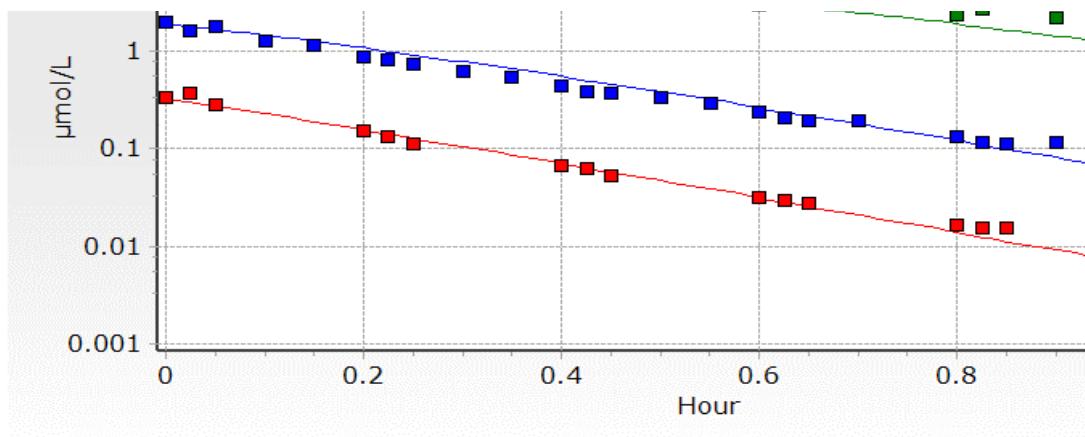
		Female		Average	95% CI
Log		Vmax	μmol/hr/mg protein	-3.58	-3.90
		Km	μmol/L	1.08	0.71

		Male		Average	95% CI
Log		Vmax	μmol/hr/mg protein	-1.99	-2.15
		Km	μmol/L	0.69	0.50

		Female		Average	95% CI
EXP		Vmax	μmol/hr/mg protein	0.028	0.020
		Km	μmol/L	2.95	2.04

		Male		Average	95% CI
EXP		Vmax	μmol/hr/mg protein	0.14	0.12
		Km	μmol/L	1.99	1.64





```

Female      gelman.dia autoburnin=FALSE)
Potential scale reduction factors:
-3.25
1.46          Point      est.      Upper      C.I.
LI           1          1
Vmax         1.01       1.02
Km           1.01       1.03

-1.87          Multivariat psrf
0.83          1.01
>
>           summary(x1)

0.039          Iterations = 6.291667
4.31           Thinning interval = 1
Number of chains = 1
Sample size per chain = 1

0.15           1 Empirical mean and standard
plus standard error of
2.29

2.50%          Mean      SD      Naive      SE
LI           0.05666  0.007222  7.61E-05  1.37E-04
Vmax         -3.57562 0.163295  1.72E-03  1.48E-02
Km           1.08021  0.188206  1.98E-03  0.017194

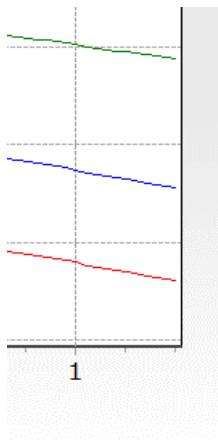
2 Quantiles for each variable:
2.50%          25%      50%      75%
LI           0.04483  0.05154  0.05588  6.09E-02
Vmax         -3.89658 -3.68692 -3.5752   -3.46475
Km           0.71304  0.95062  1.0789   1.21E+00

>           summary(x2)

Iterations = 6.291667
Thinning interval = 1
Number of chains = 1
Sample size per chain = 1

1 Empirical mean and standard
plus standard error of
2.50%          Mean      SD      Naive      SE
LI           0.05668  0.007273  7.67E-05  0.000143
Vmax         -3.60317 0.166095  1.75E-03  0.015483

```



Km 1.04806 0.191072 2.01E-03 0.017864

2 Quantiles for each variable:

	2.50%	25%	50%	75%
LI	0.04459	0.05158	0.05584	0.06108
Vmax	-3.90916	-3.72062	-3.60518	-3.48469
Km	0.6852	0.91548	1.046	1.18059

> summary(x3)

Iterations = 6.291667

Thinning interval = 1

Number of chains = 1

Sample size per chain =

1 Empirical mean and standard of plus standard error of

	Mean	SD	Naive	SE
LI	0.05663	0.007341	7.74E-05	0.000138
Vmax	-3.60558	0.16374	1.73E-03	0.01526
Km	1.04486	0.189169	1.99E-03	0.017527

2 Quantiles for each variable:

	2.50%	25%	50%	75%
LI	0.04449	0.05132	5.60E-02	0.06088
Vmax	-3.90783	-3.7177	-3.61E+00	-350.11%
Km	0.70472	0.91801	1.03063	1.1638

```

Male      gelman.dia autoburnin=FALSE)
          Potential scale reduction

          Point      est.
LI           1           1
Vmax        1.01        1.01
Km           1.01        1.01

Multivariate psrf

          1
>
>       summary(x1)

Iterations = 6.291667
Thinning interval = 
Number of chains
Sample size per

9000

deviation for each variable,
the mean:          1 Empirical mean
plus standard

Time-series SE          Mean      SD
LI           0.1513   1.24E-02
Vmax        -1.9896  6.95E-02
Km           0.6867   0.08401

          2 Quantiles for

97.50%          2.50%      25%
7.29E-02        0.1298   1.43E-01
-3.25169        -2.1464  -2.0332
1.46E+00        0.4963   6.35E-01

>       summary(x2)

Iterations = 6.291667
Thinning interval = 
Number of chains
Sample size per

9000

deviation for each variable,
the mean:          1 Empirical mean
plus standard

Time-series SE          Mean      SD
LI           0.1519   0.01272
Vmax        -1.9945  0.06455

```

Km 0.6809 0.07747

2 Quantiles for

97.50%	2.50%	25%
0.07302	LI 0.129	0.1429
-3.29035	Vmax -2.1235	-2.0368
1.41032	Km 0.5258	0.6295

> summary(x3)

Iterations = 6.291667
Thinning interval =
Number of chains
Sample size per

9000

deviation for each variable,
the mean: 1 Empirical mean
plus standard

Time-series SE

	Mean	SD
LI	0.1508	0.01253
Vmax	-1.9934	0.05477
Km	0.6822	0.06644

2 Quantiles for

97.50%	2.50%	25%
0.07309	LI 0.1287	0.1421
-326%	Vmax -2.1108	-2.0259
1.43797	Km 0.5497	0.6405

factors:

Upper C.I.

1

= 1
chain = 9000

and standard deviation for each variable,
error of the mean:

Naive SE Time-series SE
1.31E-04 0.000279
7.33E-04 0.011153
0.000886 0.013363

each variable:

50% 75% 97.50%
1.50E-01 0.1589 0.178
-1.985 -1.9403 -1.8697
6.91E-01 0.7456 0.8298

1

= 1
chain = 9000

and standard deviation for each variable,
error of the mean:

Naive SE Time-series SE
0.000134 0.000302
0.00068 0.009492

0.000817 0.011555

each variable:

50%	75%	97.50%
0.1519	0.16	0.1784
-1.9941	-1.9503	-1.872
0.6817	0.7342	0.8244

1

= 1
chain = 9000

and standard deviation for each variable,
error of the mean:

Naive	SE	Time-series SE
0.000132	0.000286	
0.000577	0.006524	
0.0007	0.008	

each variable:

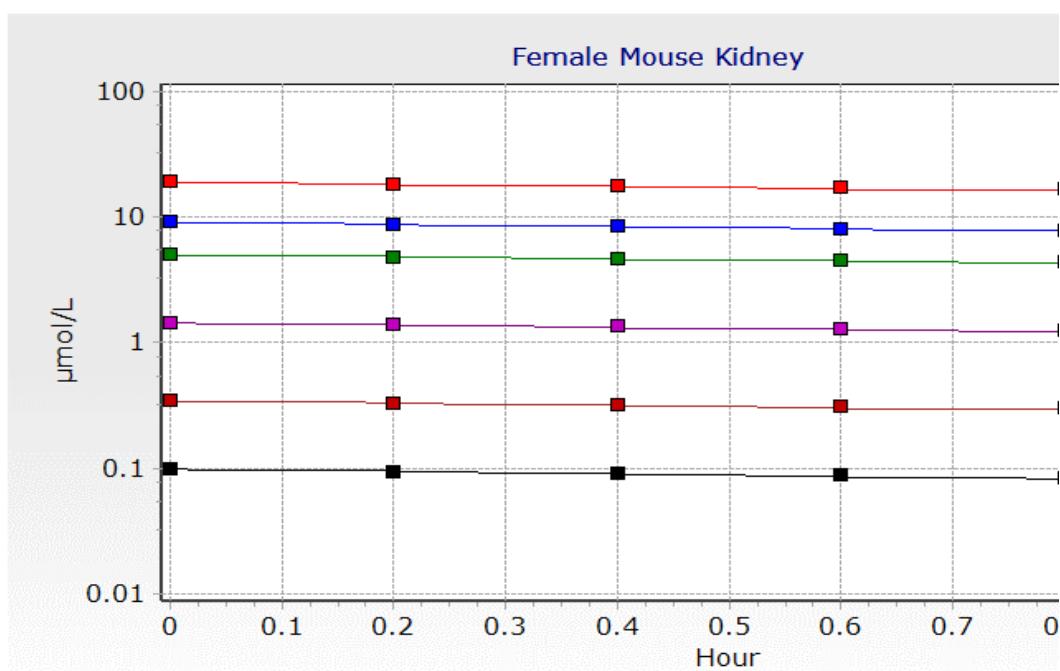
50%	75%	97.50%
0.1498	0.1586	0.1779
-1.994	-1.9569	-1.8925
0.6825	0.726	0.8042

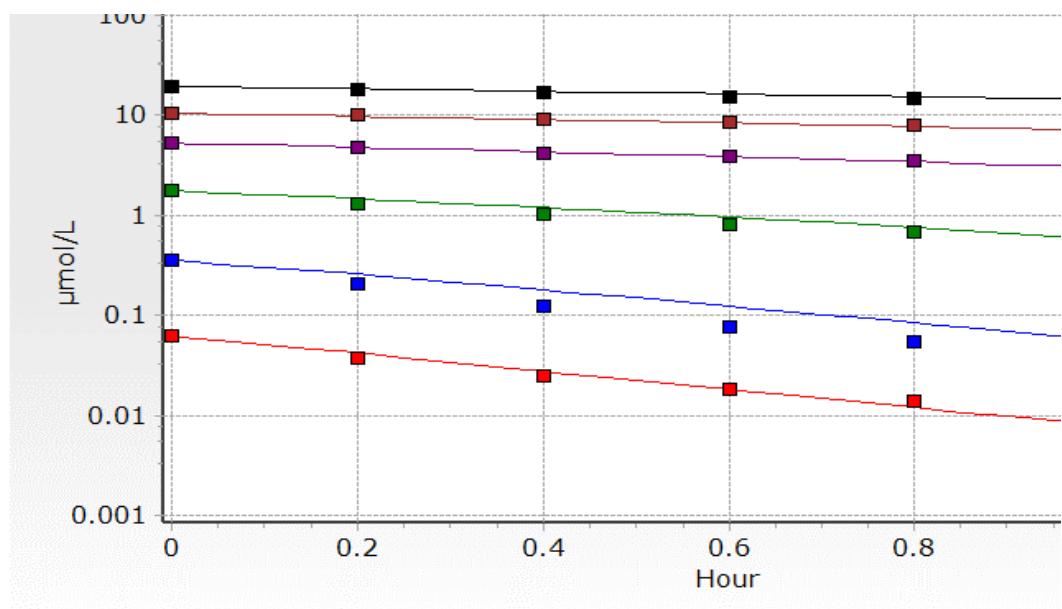
Female					
Log	VK	L/hr/mg protein	Average	95% CI	
			-7.086	-8.003	-6.528

Male					
Vmax	μmol/hr/mg protein	Average	95% CI		
Km	μmol/L	-4.58	-4.89	-4.30	
		-0.50	-0.85	-0.16	

Female					
Normal	VK	L/hr/mg protein	Average	95% CI	
Note: 2 mg of protein used in assay (VK was not scaled in the in					

Male					
Vmax	μmol/hr/mg protein	Average	95% CI		
Km	μmol/L	0.010	0.0075	0.014	
		0.61	0.43	0.85	





```

Female  gelman.dia.autoburnin=FALSE)
Potential scale reduction factors:
                                         Point      est.      Upper
LI                               1          1
VK                               1          1

Multivariate psrf

                                         1
>
>       summary(x1)

Iterations = 4.208333
Thinning interval = 1
Number of chains = 1
Sample size per chain

1 Empirical mean and
plus standard error

Mean      SD      Naive
LI       0.055  0.006865  8.86E-05
VK       -7.086 0.367382  4.74E-03

2 Quantiles for each

2.50%    25%    50%
LI       0.04316 0.05003 0.05444
VK      -800.34% -726% -703%

>       summary(x2)

Iterations = 4.208333
Thinning interval = 1
Number of chains = 1
Sample size per chain

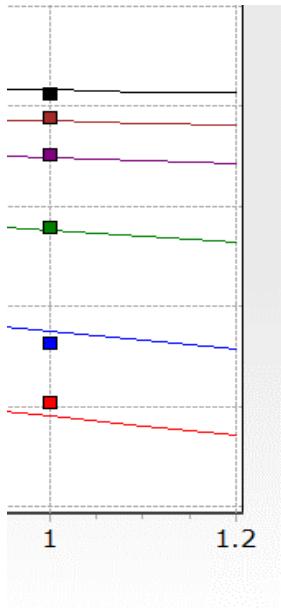
1 Empirical mean and
plus standard error

Mean      SD      Naive
LI       0.05486 0.006986 9.02E-05
VK       -7.10267 0.387496 5.00E-03

2 Quantiles for each

```

The figure shows five horizontal lines with square markers at both ends, representing quantiles for each variable. The x-axis ranges from 0.8 to 1.0.



	2.50%	25%	50%
LI	0.04288	0.05006	0.0541
VK	-8.04612	-7.29692	-7.0395

```
> summary(x3)
```

Iterations = 4.208333
 Thinning interval = 1
 Number of chains =
 Sample size per chain

1 Empirical mean and
 plus standard error

	Mean	SD	Naive
LI	0.05488	0.007194	9.29E-05
VK	-7.1014	0.378463	4.89E-03

2 Quantiles for each

	2.50%	25%	50%
LI	0.04317	0.04966	0.05401
VK	-8.09337	-7.26317	-7.02597

```

Male      gelman.dia autoburnin
          Potential scale

C.I.          Point
              LI           1
              Vmax        1.01
              Km          1.01

Multivariat psrf

              1.01
              >
              >       summary(x)

Iterations = 1
Thinning   interval
Number    of
Sample    size

1
=       6000

standard deviation for each variable,
of the mean:               1 Empirical
                           plus

SE      Time-series: SE
0.000244
0.011483

variable:               Mean
                       LI      0.1685
                           Vmax   -4.5828
                           Km     -0.5004

75%    97.50%
0.05915 0.06972
-684%  -652.75%               2 Quantiles
                                         2.50%
                                         LI      0.1334
                                         Vmax   -4.8918
                                         Km     -0.8492

>       summary(x)

1
=       6000

standard deviation for each variable,
of the mean:               Iterations =
                           Thinning interval
                           Number of
                           Sample size

SE      Time-series: SE
0.000229
0.014471

variable:               1 Empirical
                           plus
                           Mean
                           LI      0.1694
                           Vmax   -4.566

```

```

    75%   97.50%                               Km        -0.4799
0.05885 0.07025
-6.8376 -6.58109                           2 Quantiles

                                              2.50%
LI          0.1331
Vmax       -4.9056
Km         -0.8706

1
=           6000                                >       summary(x)

standard deviation for each variable,
of the mean:                                         Iterations =
SE          Time-series: SE
0.00023
0.013641                                           Thinning interval
                                                       Number of
                                                       Sample size
variable:                                            1 Empirical
                                                       plus

Mean
    75%   97.50%                               LI        0.1692
0.0593  0.07164                             Vmax     -4.596
-6.8615 -6.57264                            Km      -0.5155

2 Quantiles

                                              2.50%
LI          0.1336
Vmax       -4.943
Km         -0.9126

```

=FALSE)

reduction factors:

est.	Upper	C.I.
1	1	
1.03		
1.03		

1)

6.291667

= 1
chains = 1
per chain = 9000

mean and standard deviation for each variable,
standard error of the mean:

SD	Naive	SE	Time-series SE
0.02186	0.00023	0.0006	
0.1486	0.001566	0.016787	
0.17508	0.001846	0.019644	

for each variable:

25%	50%	75%	97.50%
0.1526	0.166	0.1817	0.2192
-4.6854	-4.5834	-4.4708	-4.3017
-0.6204	-0.5026	-0.3749	-0.1572

2)

6.291667

= 1
chains = 1
per chain = 9000

mean and standard deviation for each variable,
standard error of the mean:

SD	Naive	SE	Time-series SE
0.02201	0.000232	0.000601	
0.17121	0.001805	0.021788	

0.2016 0.002125 0.025887

for each variable:

	25%	50%	75%	97.50%
0.1541	0.1671	0.1825	0.219	
-4.6799	-4.5658	-4.4526	-4.23961	
-0.6102	-0.4888	-0.3481	-0.08956	

3)

6.291667
= 1
chains = 1
per chain = 9000

mean and standard deviation for each variable,
standard error of the mean:

SD Naive SE Time-series SE
0.02191 0.000231 0.000577
0.16421 0.001731 0.020194
0.19323 0.002037 0.023624

for each variable:

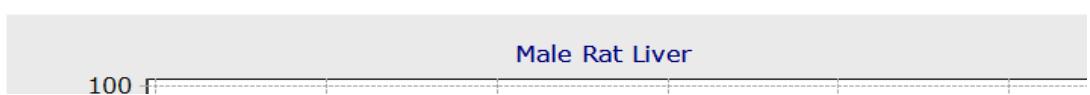
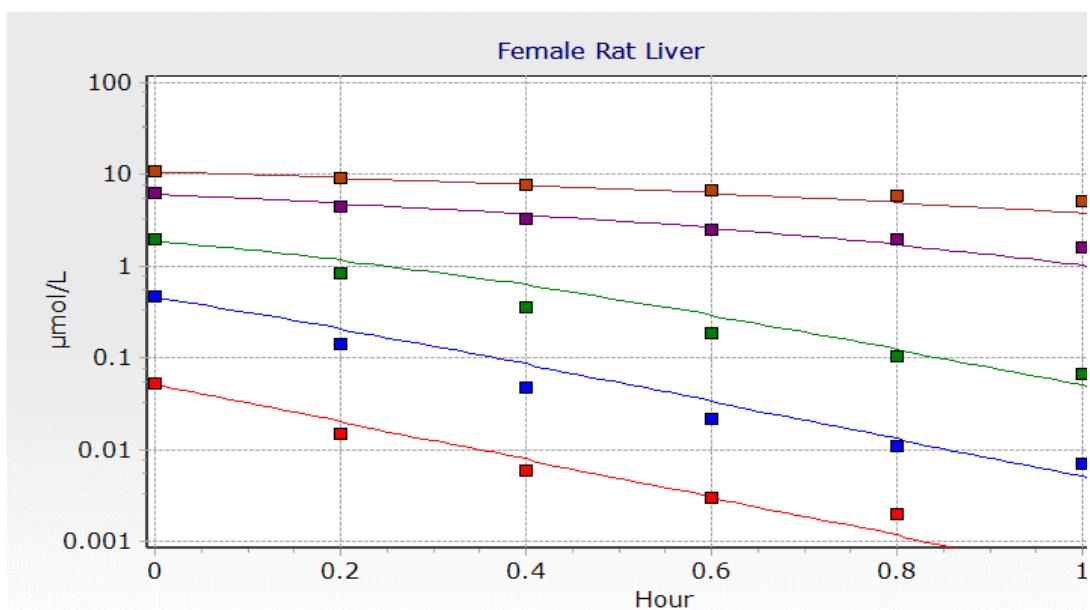
	25%	50%	75%	97.50%
0.1539	0.1673	0.1816	0.2178	
-4.6996	-4.5985	-4.4846	-4.2573	
-0.6354	-0.5188	-0.3884	-0.1192	

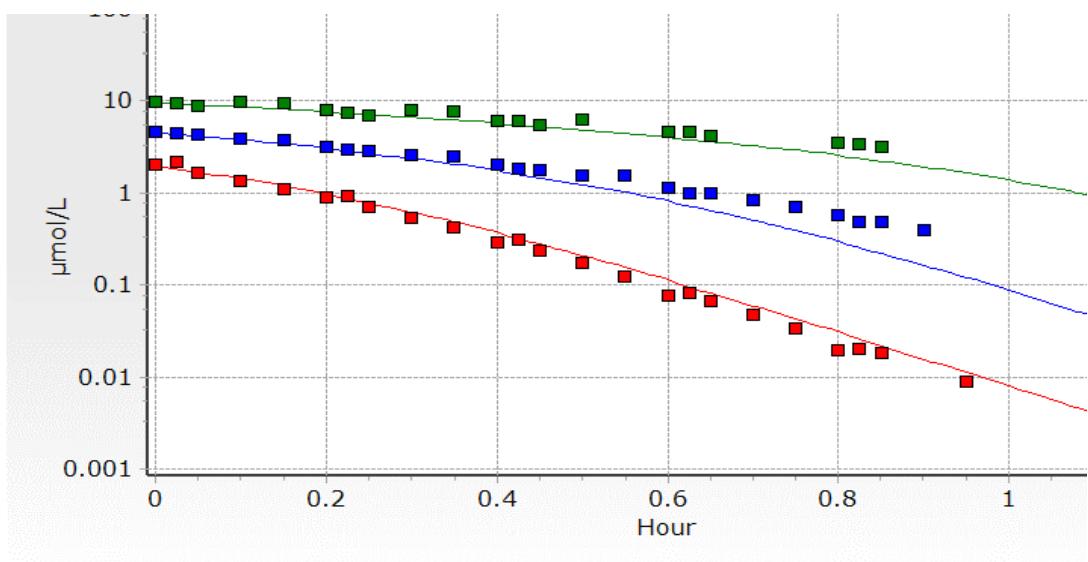
Female						
Log		Vmax	Average	95% CI		
			$\mu\text{mol/hr/mg protein}$	-2.60	-2.82	-2.39
		Km	$\mu\text{mol/L}$	-0.14	-0.41	0.13

Male					
	Vmax	Average	95% CI		-2.56
		$\mu\text{mol/hr/mg protein}$	-2.60	-2.64	
	Km	$\mu\text{mol/L}$	-0.78	-0.86	-0.70

Female						
Normal		Vmax	Average	95% CI		
			$\mu\text{mol/hr/mg protein}$	0.074	0.059	0.092
		Km	$\mu\text{mol/L}$	0.87	0.66	1.14

Male					
	Vmax	Average	95% CI		0.077
		$\mu\text{mol/hr/mg protein}$	0.074	0.071	
	Km	$\mu\text{mol/L}$	0.46	0.42	0.49





```

Female   gelman.dia autoburnin=FALSE)
Potential scale reduction factors:

          Point      est.      Upper      C.I.
LI           1         1
Vmax         1         1
Km           1         1

Multivariat psrf

1
>
>       summary(x1)

Iterations = 6.291667
Thinning interval = 1
Number of chains = 1
Sample size per chain = 9000

1 Empirical mean and standard deviation of the
               Mean     SD    Naive     SE Time-series
LI        0.3101 0.04494 0.000474 0.000858
Vmax     -2.5994 0.11139 0.001174 0.008869
Km       -0.1363 0.13676 0.001442 0.01102

2 Quantiles for each variable:

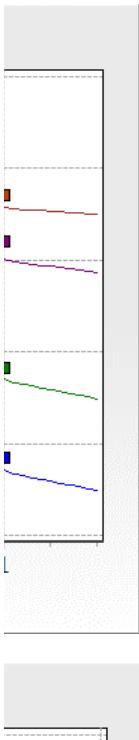
              2.50%    25%    50%    75%  97.50%
LI        0.2371 0.2784 0.3048 0.33627 0.4143
Vmax     -282.38% -267% -260% -253% -238.84%
Km       -0.4132 -0.2258 -0.1344 -0.04508 0.1285

>       summary(x2)

Iterations = 6.291667
Thinning interval = 1
Number of chains = 1
Sample size per chain = 9000

1 Empirical mean and standard deviation of the
               Mean     SD    Naive     SE Time-series
LI        0.3084 0.04487 0.000473 0.000792
Vmax     -2.5999 0.10424 0.001099 0.007707

```



```

Km      -0.1367  0.12713  0.00134  0.009361

2 Quantiles for each variable:

          2.50%    25%    50%    75%  97.50%
LI       0.2355  0.2767  0.3041  0.33364  0.4077
Vmax    -2.8157 -2.6666 -2.597   -2.5306 -2.4007
Km      -0.4001 -0.2183 -0.1358 -0.05152  0.1067

> summary(x3)

Iterations = 6.291667
Thinning interval = 1
Number of chains = 1
Sample size per chain = 9000

1 Empirical mean and standard error of the
               Mean     SD    Naive    SE Time-series
LI       0.3081  0.04542  0.000479  0.000824
Vmax    -2.5934  0.1012   0.001067  0.007662
Km      -0.1298  0.12397  0.001307  0.009401

2 Quantiles for each variable:

          2.50%    25%    50%    75%  97.50%
LI       0.2323  0.2756  0.3031  0.33434  0.4076
Vmax    -2.8046 -2.6577 -2.5932 -2.52591 -2.4032
Km      -0.3845 -0.2098 -0.1288 -0.04807  0.1093

```

Male gelman.dia autoburnin=FALSE)
Potential scale reduction factors:

	Point est.	Upper	C.I.
LI	1	1	
Vmax	1.01	1.02	
Km	1.01	1.02	

Multivariat psrf

1.01

>
> summary(x1)

Iterations = 6.291667
Thinning interval = 1
Number of chains = 1
Sample size per chain =

for each variable, 1 Empirical mean and standard
mean: plus standard error of

SE Mean SD Naive SE
LI 0.1387 0.01211 0.000128 0.000286
Vmax -2.6022 0.02094 0.000221 0.00209
Km -0.7848 0.04021 0.000424 0.003848

2 Quantiles for each variable:

2.50% 25% 50% 75%
LI 0.1181 0.1302 0.1377 0.1462
Vmax -264.36% -262% -260% -259%
Km -0.8631 -0.8127 -0.7839 -0.7582

> summary(x2)

Iterations = 6.291667
Thinning interval = 1
Number of chains = 1
Sample size per chain =

for each variable, 1 Empirical mean and standard
mean: plus standard error of

SE Mean SD Naive SE
LI 0.1389 0.01263 0.000133 0.000323
Vmax -2.603 0.02015 0.000212 0.001821

```
Km      -0.7866  0.03886  0.00041  0.003576
```

2 Quantiles for each variable:

	2.50%	25%	50%	75%
LI	0.117	0.1302	0.1377	0.1469
Vmax	-2.6444	-2.6161	-2.602	-2.5894
Km	-0.8671	-0.8121	-0.7847	-0.7607

```
> summary(x3)
```

Iterations = 6.291667
Thinning interval = 1
Number of chains = 1
Sample size per chain =

for each variable, 1 Empirical mean and standard
mean: plus standard error of

	Mean	SD	Naive	SE
LI	0.1391	0.01267	0.000134	0.000302
Vmax	-2.6059	0.02275	0.00024	0.002281
Km	-0.7919	0.04361	0.00046	0.004511

2 Quantiles for each variable:

	2.50%	25%	50%	75%
LI	0.1163	0.1301	0.1381	0.1471
Vmax	-2.6539	-2.6204	-2.603	-2.5906
Km	-0.8854	-0.8192	-0.7875	-0.763

9000

deviation for each variable,
the mean:

Time-series SE

97.50%

0.1655

-256.15%

-0.7032

9000

deviation for each variable,
the mean:

Time-series SE

97.50%
0.1653
-2.5655
-0.7141

9000

deviation for each variable,
the mean:

Time-series SE

97.50%
0.1663
-2.5661
-0.7161

Female

			Median	95% CI
Log	VK	L/hr/mg protein	-9.0117	-9.9544 -7.6178

Male

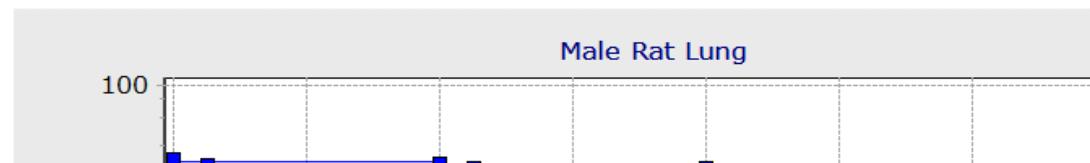
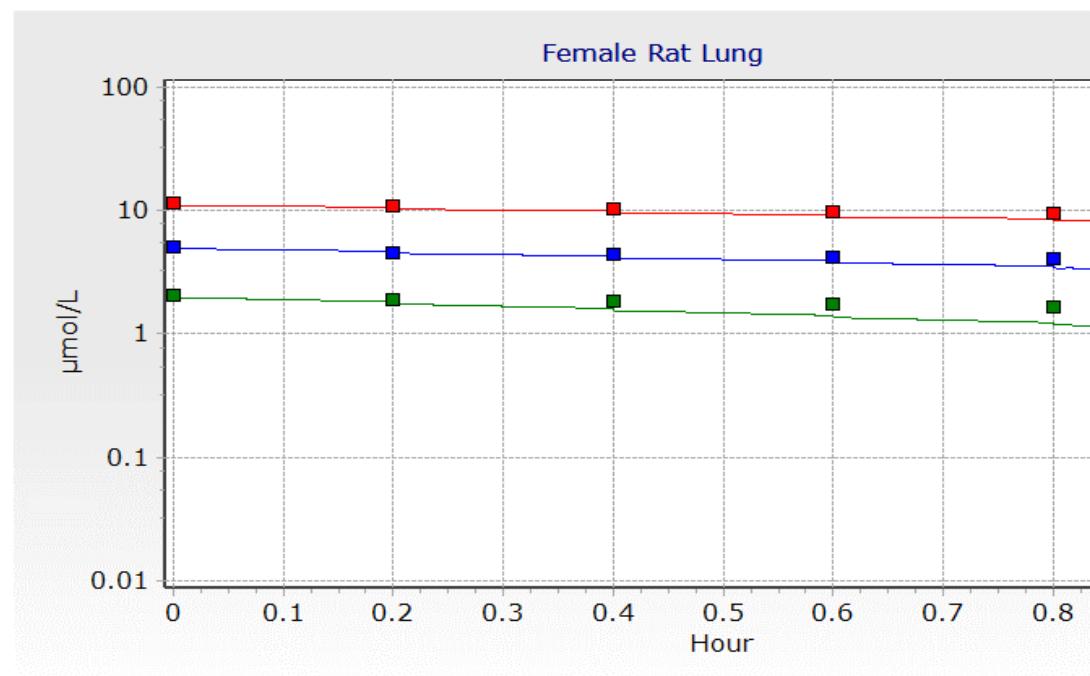
			Median	95% CI
VK	L/hr/mg protein	-8.2990	-9.8938 -6.4870	

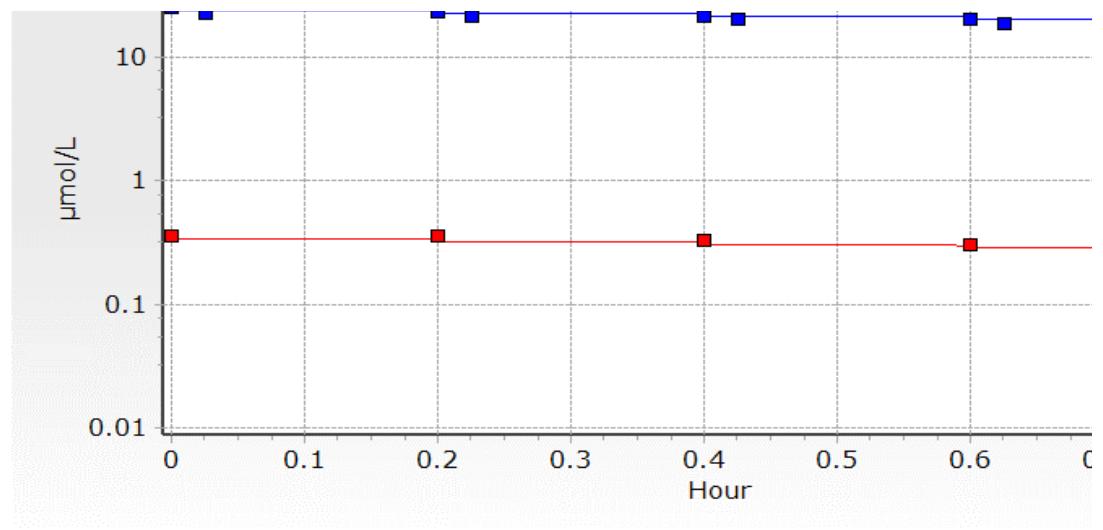
Female

			Median	95% CI
EXP	VK	L/hr/mg protein	0.00012	0.000048 0.00049

Male

			Median	95% CI
VK	L/hr/mg protein	0.00025	0.000050 0.0015	





```
Female    gelman.dia autoburnin=FALSE)
Potential scale reduction
```

	Point est.
LI	1.53 2.35
VK	1 1.01

Multivariate psrf

1.43

```
>
>      summary(x1)
```

```
Iterations = 6.291667
Thinning interval =
Number of chains
Sample size per
```

1 Empirical mean
plus standard

	Mean	SD
LI	0.06347	0.01215
VK	-9.01169	0.66135

2 Quantiles for

	2.50%	25%
LI	0.04525	0.05461
VK	-9.95444	-9.56155

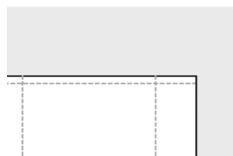
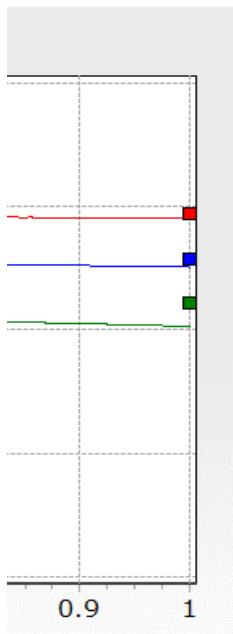
```
>      summary(x2)
```

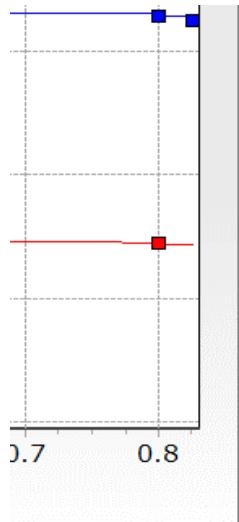
```
Iterations = 6.291667
Thinning interval =
Number of chains
Sample size per
```

1 Empirical mean
plus standard

	Mean	SD
LI	0.08538	0.0158
VK	-8.97361	0.6625

2 Quantiles for





	2.50%	25%
LI	0.06059	0.07447
VK	-9.95077	-9.52827

```
> summary(x3)
```

Iterations = 6.291667
 Thinning interval =
 Number of chains
 Sample size per

1 Empirical mean
 plus standard

	Mean	SD
LI	0.06975	0.01289
VK	-9.04204	0.64275

2 Quantiles for

	2.50%	25%
LI	0.05008	0.06028
VK	-9.95087	-9.57765

factors:
 male gelman.dia autoburnin
 Potential scale
 Upper C.I. Point
 LI 1.05
 VK 1

Multivariat psrf
 1.05
 >
 > summary(x

Iterations =
 Thinning interval
 Number of
 Sample size
 1
 = 1
 chain = 9000

and standard deviation for each variable,
 error of the mean: 1 Empirical plus

Naive SE Time-serie:SE Mean
 1.28E-04 0.000317 LI 0.09726
 6.97E-03 0.016355 VK -8.29902

each variable: 2 Quantiles
 50% 75% 97.50% 2.50%
 6.16E-02 0.06998 0.09222 LI 0.06738
 -9.11E+00 -8.54981 -7.61775 VK -9.8938

> summary(x

Iterations =
 Thinning interval
 Number of
 Sample size
 1
 = 1
 chain = 9000

and standard deviation for each variable,
 error of the mean: 1 Empirical plus

Naive SE Time-serie:SE Mean
 1.67E-04 0.00041 LI 0.08723
 6.98E-03 0.016457 VK -8.29621

each variable: 2 Quantiles

50%	75%	97.50%		2.50%
0.08306	0.09466	0.1227	LI	0.05936
-9.02428	-8.53394	-7.5273	VK	-9.88474
> summary(x)				
1.00E+00			Iterations	=
=	1		Thinning	interval
chain	=	9000	Number	of
and	standard	deviation	Sample	size
error	of	for		
	the	each		1 Empirical
	mean:	variable,		plus
Naive	SE	Time-series SE		Mean
1.36E-04	0.000322		LI	0.09023
6.78E-03	0.016838		VK	-8.30696
each	variable:			2 Quantiles
50%	75%	97.50%		2.50%
0.06819	0.07688	0.09919	LI	0.06286
-9.12562	-8.60806	-7.59563	VK	-9.90864

=FALSE)

reduction factors:

est.	Upper	C.I.
1.17		
	1	

1)

6.291667

= 1
chains = 1
per chain = 9000

mean and standard deviation for each variable,
standard error of the mean:

SD	Naive	SE	Time-series SE
0.02029	0.000214	0.000497	
0.96116	0.010132	0.020162	

for each variable:

25%	50%	75%	97.50%
0.08271	0.0941	0.109	0.1451
-9.08695	-8.3304	-7.562	-6.487

2)

6.291667

= 1
chains = 1
per chain = 9000

mean and standard deviation for each variable,
standard error of the mean:

SD	Naive	SE	Time-series SE
0.01804	0.00019	0.000477	
0.93838	0.009891	0.018407	

for each variable:

25%	50%	75%	97.50%
0.07423	0.0843	0.09709	0.1313
-9.06282	-8.2922	-7.59829	-6.5136

3)

6.291667
= 1
chains = 1
per chain = 9000

mean and standard deviation for each variable,
standard error of the mean:

SD	Naive	SE	Time-series SE
0.01964	0.000207	0.000509	
0.95723	0.01009	0.018776	

for each variable:

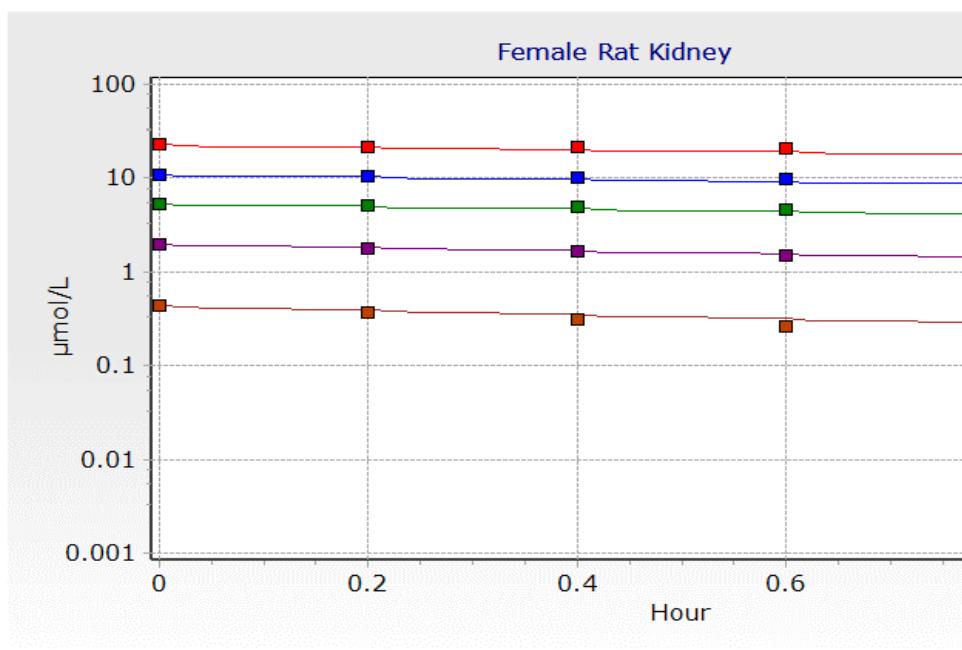
25%	50%	75%	97.50%
0.07608	0.08625	0.1011	0.1369
-9.08093	-8.31774	-7.5409	-6.5362

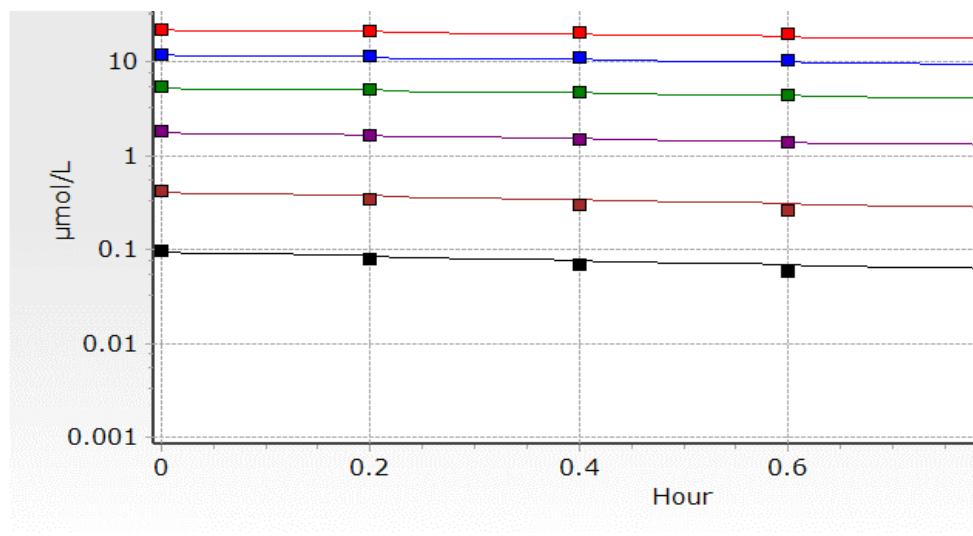
Female					
Log			Average	95% CI	
	Vmax	µmol/hr/r	-5.635	-5.887	-5.37
	Km	µmol/L	-0.568	-0.875	-0.25

Male					
Log			Average	95% CI	
	Vmax	µmol/hr/r	-5.51	-5.77	-5.30
	Km	µmol/L	-0.17	-0.47	0.08

Female					
Normal			Average	95% CI	
	Vmax	µmol/hr/r	0.0036	0.0028	0.0046
	Km	µmol/L	0.57	0.42	0.78

Male					
Normal			Average	95% CI	
	Vmax	µmol/hr/r	0.0040	0.0031	0.0050
	Km	µmol/L	0.84	0.63	1.08





```
Female gelman.dia autoburnin=FALSE)
Potential scale reduction factors:
```

	Point est.	Upper
LI	1	1
Vmax	1.01	1.01
Km	1.01	1.01

Multivariat psrf

```
1
>
> summary(x1)
```

```
Iterations = 6.291667
Thinning interval = 1
Number of chains = 
Sample size per chain
```

1 Empirical mean and
plus standard error

	Mean	SD	Naive
LI	0.05143	0.006376	6.72E-05
Vmax	-5.63477	0.128699	1.36E-03
Km	-0.56835	0.156828	1.65E-03

2 Quantiles for each

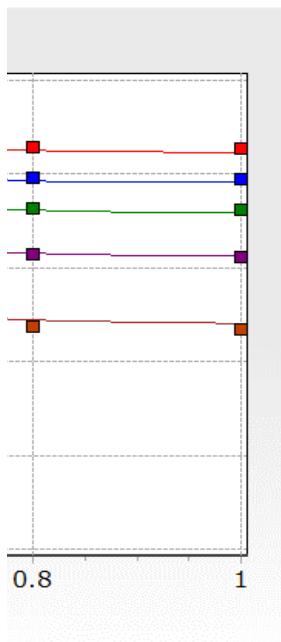
	2.50%	25%	50%
LI	0.04073	0.04691	0.05095
Vmax	-5.8872	-5.72014	-5.63855
Km	-0.87512	-0.671	-0.57188

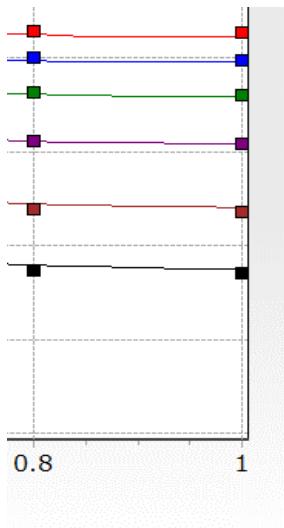
```
> summary(x2)
```

```
Iterations = 6.291667
Thinning interval = 1
Number of chains = 
Sample size per chain
```

1 Empirical mean and
plus standard error

	Mean	SD	Naive
LI	0.05171	0.006862	7.23E-05
Vmax	-5.61889	0.152421	1.61E-03





Km -0.54824 0.187093 1.97E-03

2 Quantiles for each

	2.50%	25%	50%
LI	0.04048	0.04687	0.05109
Vmax	-5.90398	-5.71753	-5.62157
Km	-0.89727	-0.66845	-0.55158

> summary(x3)

Iterations = 6.291667
 Thinning interval = 1
 Number of chains =
 Sample size per chain

1 Empirical mean and
 plus standard error

	Mean	SD	Naive
LI	0.0516	0.00645	6.80E-05
Vmax	-5.6284	0.14545	1.53E-03
Km	-0.5598	0.17817	1.88E-03

2 Quantiles for each

	2.50%	25%	50%
LI	0.04073	0.04713	0.05096
Vmax	-5.89818	-5.72928	-5.63684
Km	-0.88891	-0.68574	-0.57018

Male gelman.dia autoburnin
 Potential scale

C.I. Point
 LI 1
 Vmax 1
 Km 1

Multivariat psrf

1
 >
 > summary(x)

Iterations =
 Thinning interval
 Number of
 Sample size

1
 = 9000

standard deviation for each variable,
 of the mean: 1 Empirical plus

SE Time-serie: SE Mean
 0.000115 LI 0.0366
 0.009781 Vmax -5.5099
 0.01198 Km -0.1708

variable: 2 Quantiles

75% 97.50% 2.50%
 0.05528 0.06586 LI 0.02872
 -5.54868 -5.37112 Vmax -5.76535
 -0.46503 -0.24627 Km -0.46827

> summary(x)

Iterations =
 Thinning interval
 Number of
 Sample size

1
 = 9000

standard deviation for each variable,
 of the mean: 1 Empirical plus

SE Time-serie: SE Mean
 0.000131 LI 0.0367
 0.014266 Vmax -5.5169

0.017212 Km -0.1787

variable: 2 Quantiles

75%	97.50%	2.50%
0.0556	0.06724	LI 0.02917
-5.5261	-5.29947	Vmax -5.76235
-0.4331	-0.15516	Km -0.46972

> summary(x)

Iterations =
Thinning interval
Number of
Sample size

1
= 9000

standard deviation for each variable,
of the mean: 1 Empirical
plus

SE	Time-series: SE	Mean
0.000117		LI 0.03701
0.012839		Vmax -5.50936
0.015631		Km -0.17063

variable: 2 Quantiles

75%	97.50%	2.50%
0.05543	0.06643	LI 0.02885
-5.53277	-5.3281	Vmax -5.77204
-0.44269	-0.19407	Km -0.49261

=FALSE)

reduction factors:

est.	Upper	C.I.
	1.01	
	1.01	
	1.01	

1)

6.291667
= 1
chains = 1
per chain = 9000

mean and standard deviation for each variable,
standard error of the mean:

SD	Naive	SE	Time-series SE
0.00458	4.83E-05	0.000115	
0.11633	1.23E-03	0.013289	
0.13986	1.47E-03	0.015572	

for each variable:

	25%	50%	75%	97.50%
0.03337	0.03626	0.03945	0.04719	
-5.58805	-5.50115	-5.42904	-5.30174	
-0.26657	-0.16015	-0.07087	0.08044	

2)

6.291667
= 1
chains = 1
per chain = 9000

mean and standard deviation for each variable,
standard error of the mean:

SD	Naive	SE	Time-series SE
0.004544	4.79E-05	0.000114	
0.124218	1.31E-03	0.014725	

0.150492 1.59E-03 0.01796

for each variable:

	25%	50%	75%	97.50%
0.03349	0.03625	0.0395	0.04692	
-5.59706	-5.51918	-5.43185	-5.26703	
-0.27497	-0.18355	-0.07704	0.12111	

3)

6.291667

= 1
chains = 1
per chain = 9000

mean and standard deviation for each variable,
standard error of the mean:

SD	Naive	SE	Time-series SE
0.00484	5.10E-05	0.000119	
0.13269	1.40E-03	0.017143	
0.16124	1.70E-03	0.022123	

for each variable:

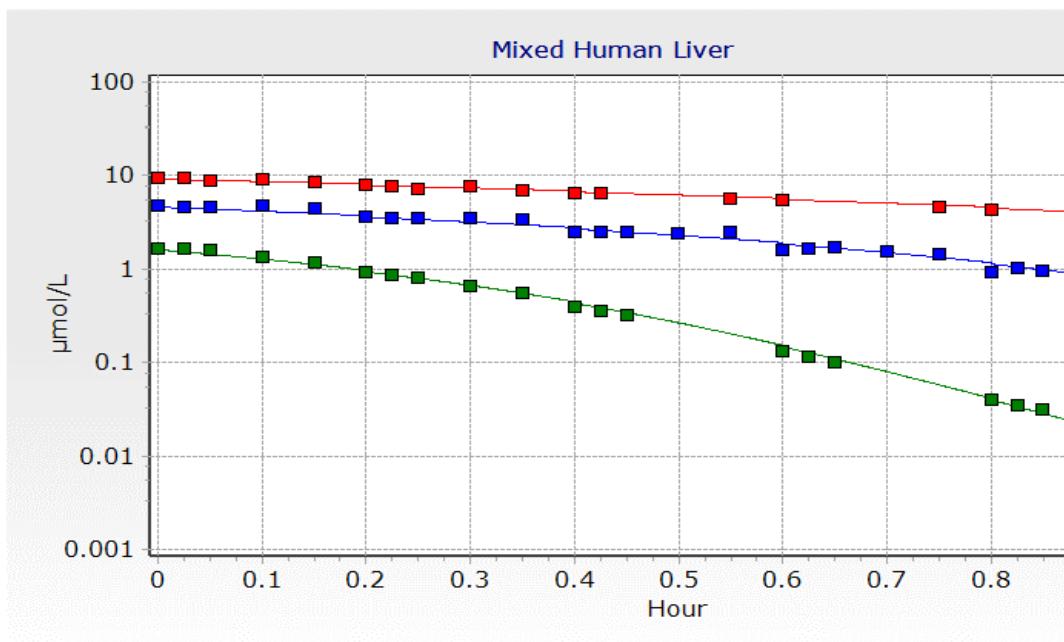
	25%	50%	75%	97.50%
0.03364	0.03654	0.03996	0.04769	
-5.6047	-5.51136	-5.41381	-5.26598	
-0.28763	-0.17486	-0.05456	0.13018	

Mixed Human

Log	Vmax	Average	95% CI	
		$\mu\text{mol}/\text{hr}/\text{m}$	-2.932	-2.966
Km	$\mu\text{mol}/\text{L}$	-0.960	-1.033	-0.89

Mixed Human

EXP	Vmax	Average	95% CI	
		$\mu\text{mol}/\text{hr}/\text{m}$	0.053	0.052
Km	$\mu\text{mol}/\text{L}$	0.38	0.36	0.41




```
gelman.dia autoburnin=FALSE)
Potential scale reduction factors:
```

	Point est.	Upper	C.I.
LI	1	1	
Vmax	1	1.01	
Km	1	1.01	

Multivariat psrf

```
1
>
> summary(x1)

Iterations = 6.291667
Thinning interval = 1
Number of chains = 1.00E+00
Sample size per chain = 9.00E+03

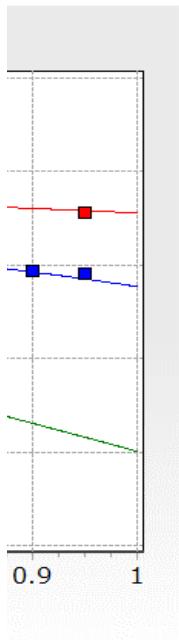
1 Empirical mean and standard error of the
               Mean      SD    Naive      SE Time-series
LI       0.07742 0.007129 7.52E-05 0.000179
Vmax    -2.93233 0.017557 1.85E-04 0.001708
Km      -0.96031 0.036443 3.84E-04 0.003462

2 Quantiles for each variable:
               2.50%     25%     50%     75%   97.50%
LI       0.06495 0.07252 0.07689 0.08134 0.09336
Vmax    -2.96584 -2.94408 -2.93286 -2.92034 -2.89914
Km      -1.03345 -0.98589 -0.96104 -9.35E-01 -8.89E-01

> summary(x2)

Iterations = 6.291667
Thinning interval = 1
Number of chains = 1
Sample size per chain = 9000

1 Empirical mean and standard error of the
               Mean      SD    Naive      SE Time-series
LI       0.07727 0.007385 7.78E-05 0.00019
Vmax    -2.93145 0.017251 1.82E-04 0.001639
```



Km -0.95854 0.035921 3.79E-04 0.003448

2 Quantiles for each variable:

	2.50%	25%	50%	75%	97.50%
LI	0.06391	0.07213	0.07686	0.08188	0.0931
Vmax	-2.96638	-2.94276	-2.93131	-2.91955	-2.8979
Km	-1.03145	-0.98261	-0.95757	-0.93321	-0.8917

> summary(x3)

Iterations = 6.291667
Thinning interval = 1
Number of chains = 1
Sample size per chain = 9000

1 Empirical mean and standard error of the
Mean SD Naive SE Time-series
LI 0.07724 0.007155 7.54E-05 0.00017
Vmax -2.93312 0.018329 1.93E-04 0.001808
Km -0.96205 0.038153 4.02E-04 0.004022

2 Quantiles for each variable:

	2.50%	25%	50%	75%	97.50%
LI	0.06509	0.07217	7.66E-02	0.0816	0.09303
Vmax	-2.96642	-2.94553	-2.94E+00	-2.9204	-2.89454
Km	-1.03127	-0.99049	-0.96502	-0.9344	-0.88352

for each variable,
mean:

SE

for each variable,
mean:

SE

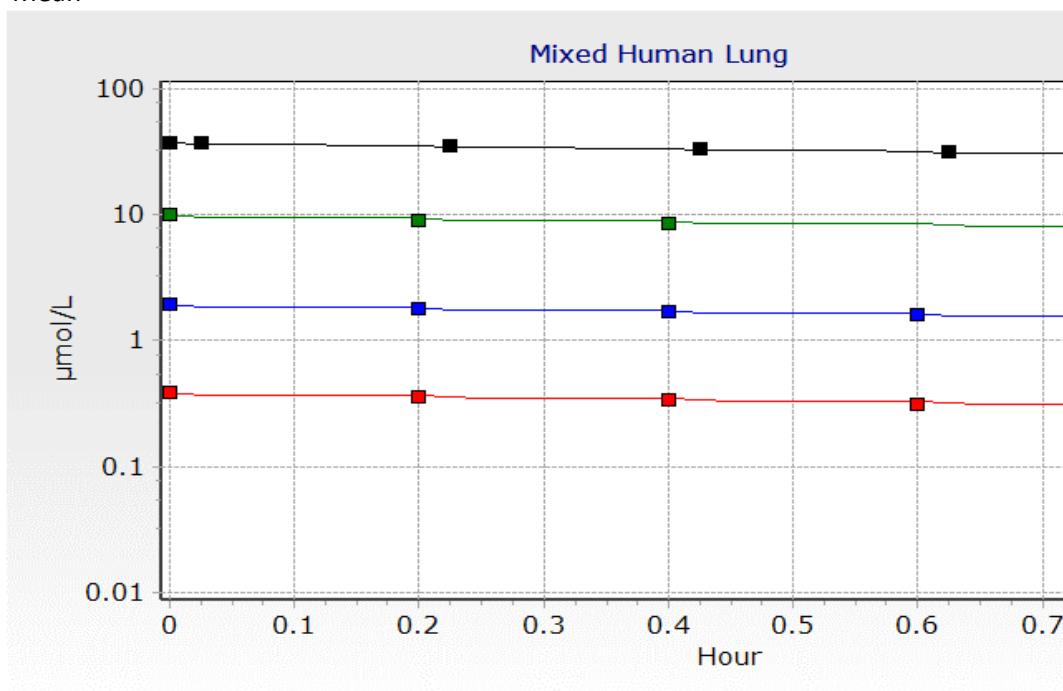
for each variable,
mean:

SE

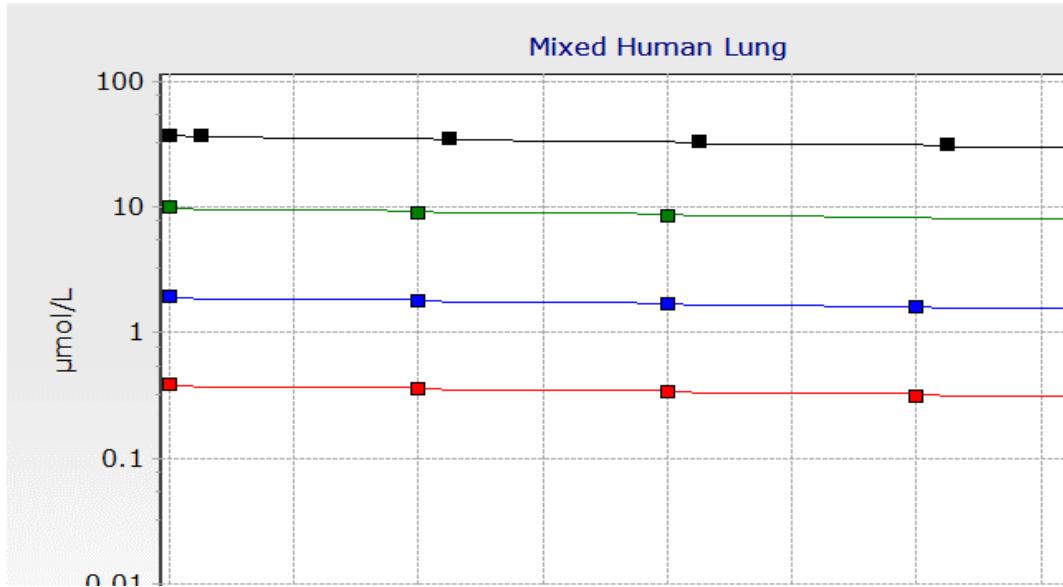
		Mixed Human Lung Microsomes	
		Mean	95% CI
Log	VK	L/hr/mg protein	-31.84 -57.85

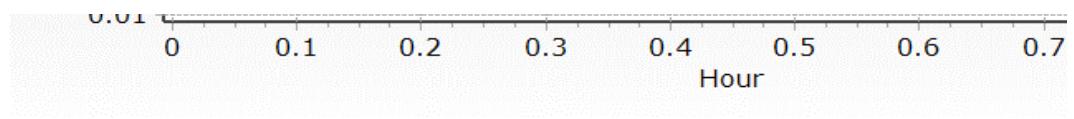
		Mixed	
		Mean	95% CI
EXP	VK	L/hr/mg protein	1.49E-14 7.53E-26

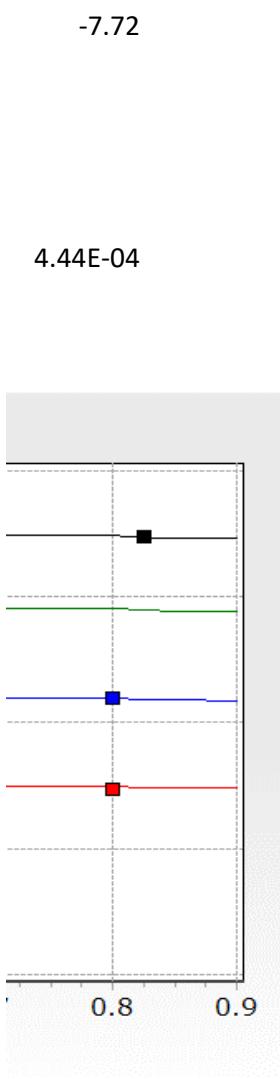
Mean



Upper 95th percentile







```
gelman.dia autoburnin
Potential scale
```

	Point
LI	1.04
VK	1

```
Multivariat psrf
1.04
>
> summary(x
```

```
Iterations =
Thinning interval
Number of
Sample size
```

```
1 Empirical
plus
```

```
Mean
LI 174.80%
VK -31.84
```

```
2 Quantiles
```

```
2.50%
LI 1.299
VK -57.848
```

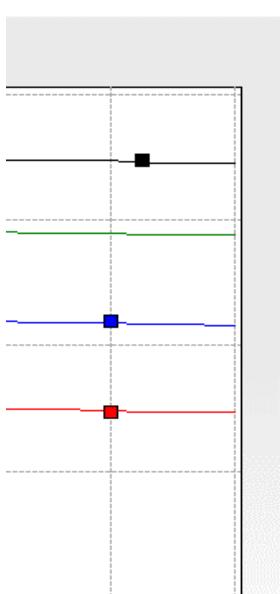
```
> summary(x
```

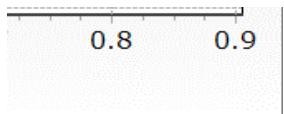
```
Iterations =
Thinning interval
Number of
Sample size
```

```
1 Empirical
plus
```

```
Mean
LI 1.869
VK -32.531
```

```
2 Quantiles
```





2.50%
LI 1.396
VK -57.812

> summary(x)

Iterations =
Thinning interval
Number of
Sample size

1 Empirical
plus

Mean
LI 1.768
VK -31.91

2 Quantiles

2.50%
LI 1.322
VK -57.812

=FALSE)

reduction factors:

est.	Upper	C.I.
1.12		
	1	

1)

6.291667

= 1.00E+00
chains = 1.00E+00
per chain = 9000

mean and standard deviation for each variable,
standard error of the mean:

SD	Naive	SE	Time-series SE
28%	0%	0%	
14.73	0.15527	0.299403	

for each variable:

	25%	50%	75%	97.50%
	1.552	1.715	1.91	2.379
	-43.943	-31.575	-19.39	-7.719

2)

6.291667

= 1.00E+00
chains = 1
per chain = 9000

mean and standard deviation for each variable,
standard error of the mean:

SD	Naive	SE	Time-series SE
0.2964	0.003125	0.005359	
14.5411	0.153276	0.293089	

for each variable:

25%	50%	75%	97.50%
1.658	1.832	2.039	2.543
-44.328	-32.664	-20.58	-7.755

3)

6.291667
= 1
chains = 1
per chain = 9000

mean and standard deviation for each variable,
standard error of the mean:

SD	Naive	SE	Time-series SE
0.2825	0.002977	0.004857	
14.6297	0.154211	0.282274	

for each variable:

25%	50%	75%	97.50%
1.561	1.74	1.93	2.409
-43.854	-31.83	-19.52	-7.584

MCMC Mean Parameters

Kg estimated			Liver			Lung			Kidney		
			Mean	95% CI		Mean	95% CI		Mean	95% CI	
Male Mouse	Vmax (μmol/hr/mg protein)	0.25	0.24	0.26		0.14	0.12	0.15		0.010	0.008
	Km (μmol/L)	0.99	0.89	1.09		1.99	1.64	2.29		0.61	0.43
	Female Mouse	0.11	0.093	0.14		0.028	0.020	0.039		0.00042	0.00017
Male Rat	Km (μmol/L)	0.63	0.44	0.90		2.95	2.04	4.31		0.84	0.63
	Vk (L/hr/mg protein)									0.0040	0.0031
	Vmax (μmol/hr/mg protein)	0.074	0.071	0.077		0.00025	0.000050	0.0015		0.0050	0.0050
Female Rat	Km (μmol/L)	0.46	0.42	0.49		0.00012	0.000048	0.00049		0.57	0.42
	Vk (L/hr/mg protein)	0.074	0.059	0.092						0.0036	0.0028
	Vmax (μmol/hr/mg protein)	0.87	0.66	1.14						0.78	0.78
Human	Km (μmol/L)	0.053	0.052	0.055		7.62E-05				Not Measured	
	Vk (L/hr/mg protein)	0.38	0.36	0.41		0.38					
	Vk (L/hr/mg protein)	1.49E-14	7.53E-26	4.44E-04		1.99E-04					
Note: Flux was estimated for male mouse liver incubation - Km was fixed at 1.0 while Vmax and Kg were included in the calibration - see output below and on worksheet Male_Mouse_Liver_Kg (Using A1) Vk (L/hr/mg protein)											

MCMC Mean Parameters

Kg estimated using the male mouse liver in vitro data (most informative)

		Liver		
		Mean	95% CI	
Male Mouse	Vmax (μmol/hr/mg protein)	0.25	0.24	0.26
	Km (μmol/L)	1.00		
	Kgi	0.45	0.34	0.65

Summary In Vivo Parameters

Liver		
Male Mouse	Vmax (mg/hr/BW^{0.75})	18.99
	Km (mg/L)	0.088
Female Mouse	Vmax (mg/hr/BW^{0.75})	8.33
	Km (mg/L)	0.055
	KFKIC (L/hr/kg BW)	
Male Rat	Vmax (mg/hr/BW^{0.75})	7.87
	Km (mg/L)	0.040
	KFLUC (L/hr/kg BW)	
Female Rat	Vmax (mg/hr/BW^{0.75})	7.30
	Km (mg/L)	0.077
	KFLUC (L/hr/kg BW)	
Human	Vmax (mg/hr/BW^{0.75})	17.53
	Km (mg/L)	0.034
(Using A1)	KFLUC (L/hr/kg BW)	
(Upper 95% CI)	KFLUC (L/hr/kg BW)	

KFLUC and KFKIC are scaled to tissue volume - value here is scaled and multiplied by BW in the model file

Revised Scaling

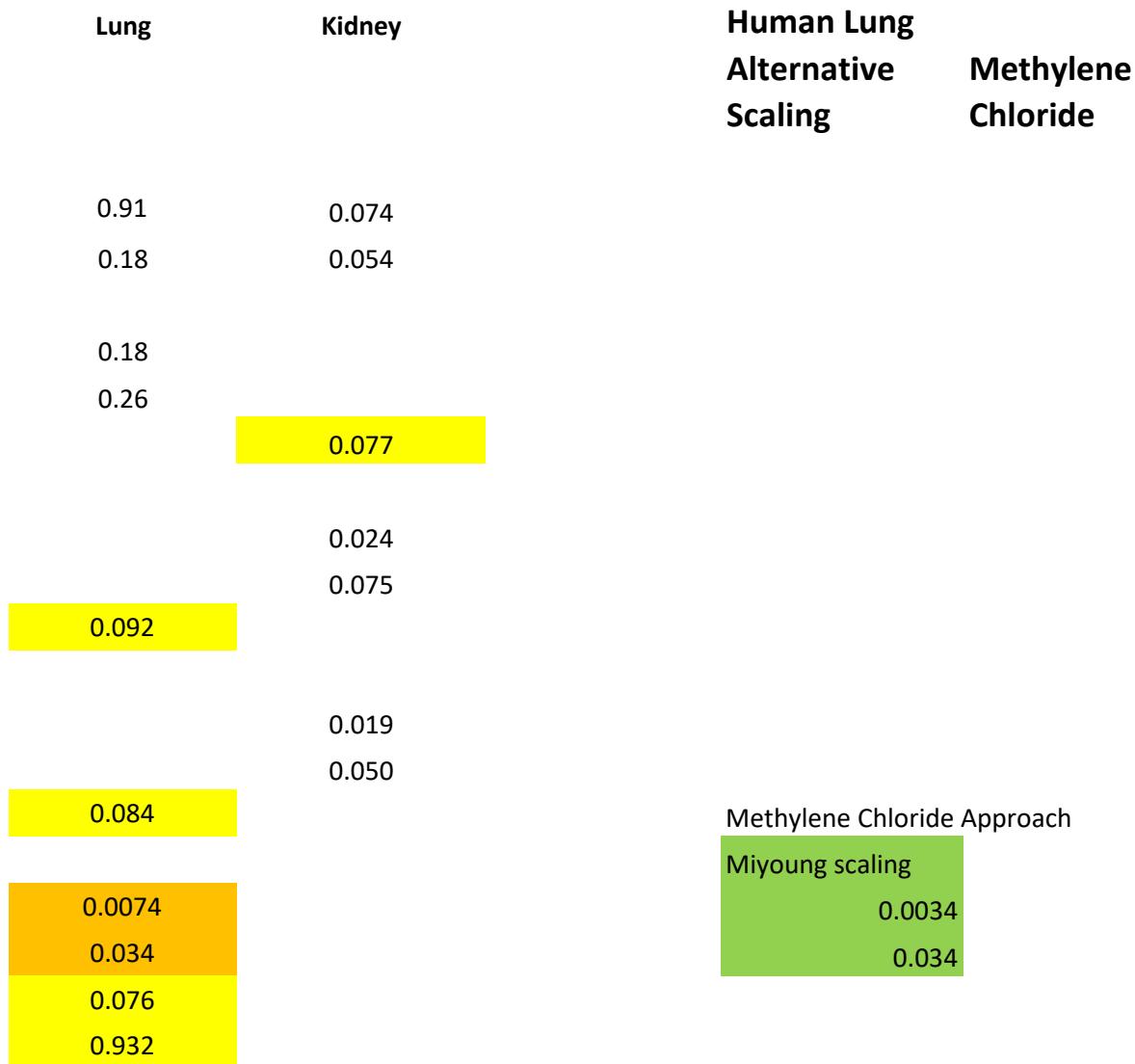
Scaling factors for average adults in each species	Parameter	BW (kg)	Liver fractional weight (VLC)	Lung fractional weight (VLUC)
	B6C3F1 Mouse (Female)	0.035	0.0549	0.0073
	B6C3F1 Mouse (Male)	0.04	0.0549	0.0073
	F344 Rat (Female)	0.33	0.0366	0.005
	F344 Rat (Male)	0.45	0.0366	0.005
	Average Human	70	0.0257	0.0076
	Reference	Brown et al, 1997 (page 415 in text)	Brown et al, 1997 (Tables 4, 5, & 7)	Brown et al, 1997 (Tables 4, 5, & 7)

References

1. Brown et al., 1997, Toxicol. Ind. Health, July-Aug;13(4):407-84. Re
2. Barter et al., Drug Metab Dispos. 2008 Dec;36(12):2405-9. doi: 10
3. Himmelstein et al., Toxicol Sci. 2004b May;79(1):28-37. Epub 200
4. Houston and Galetin, Curr Drug Metab. 2008 Nov;9(9):940-51. Re

5. Scotcher et al., Drug Metab Dispos. 2017 May;45(5):556-568. doi:





I to fraction of tissue volume represented by the tissue

Kidney fractional weight (VKC)	Liver mg microsomal protein per g liver (MPPGL)	Lung mg microsomal protein per g lung (MPPGLU)	Kidney mg microsomal protein per g kidney (MPPGK)	MW
0.0167	35	23	11	88.53650
0.0167	35	23	11	g/mol = ug/umol
0.0073	40	23	11	
0.0073	40	23	11	
0.0044	50	23	11	
Brown et al, 1997 (Tables 4, 5, & 7)	Houston and Galetin, 2008 for rat; Barter et al., 2008 for human; rat value used for mouse	Same as Himmelstein et al., 2004b	Based on Scotcher et al., 2017	

Review. PubMed PMID:9249929

).1124/dmd.108.021311. Epub 2008 Sep 5. PubMed PMID: 18775982.

4 Feb 19. PubMed PMID: 14976335.

Review. PubMed PMID: 18991591.

Biological Scaling	Vmaxc (mg/h/kg BW ^{0.75})
Female Mouse	Values
LIVER	Scaling & calculation
	Unit

Biological Scaling	Vmaxc (mg/h/kg BW ^{0.75})
Male Mouse	Values
LIVER	Scaling & calculation
	Unit

Biological Scaling	Vmaxc (mg/h/kg BW ^{0.75})
Female Rat	Values

LIVER	Scaling & calculation
	Unit

Biological Scaling	Vmaxc (mg/h/kg BW ^{0.75})
Male Rat	Values
LIVER	Scaling & calculation
	Unit

Biological Scaling	Vmaxc (mg/h/kg BW ^{0.75})
Mixed gender Human	Values
LIVER	Scaling & calculation
	Unit

In Vitro Value	x Scaling factor	x Tissue weight	/BW ^{0.75}	x MW = In vivo parameter (unit in PBPK model)
0.11	35.00	7.61	94.07	8.33
	x MPPGL (mg MP/g liver)	x BW (kg) x VLC x 1000 (g/kg)	/BW ^{0.75}	x MW (ug/umol)/1000 (ug/mg)
umol/h/mg MP	umol/h/g liver	umol/h	umol/h/kg BW ^{0.75}	mg/h/kg BW ^{0.75}

In Vitro Value	x Scaling factor	x Tissue weight	/BW ^{0.75}	x MW = In vivo parameter (unit in PBPK model)
0.25	35.00	19.19	214.51	18.99
	x MPPGL (mg MP/g liver)	x BW (kg) x VLC x 1000 (g/kg)	/BW ^{0.75}	x MW (ug/umol)/1000 (ug/mg)
umol/h/mg MP	umol/h/g liver	umol/h	umol/h/kg BW ^{0.75}	mg/h/kg BW ^{0.75}

In Vitro Value	x Scaling factor	x Tissue weight	/BW ^{0.75}	x MW = In vivo parameter (unit in PBPK model)
0.074	40.00	35.90	82.46	7.30

	x MPPGL (mg MP/g liver)	x BW (kg) x VLC x 1000 (g/kg)	/BW ^{0.75}	x MW (ug/umol)/1000 (ug/mg)
umol/h/mg MP	umol/h/g liver	umol/h	umol/h/kg BW ^{0.75}	mg/h/kg BW ^{0.75}

In Vitro Value	x Scaling factor	x Tissue weight	/BW ^{0.75}	x MW = In vivo parameter (unit in PBPK model)
0.074	40.00	48.82	88.86	7.87
	x MPPGL (mg MP/g liver)	x BW (kg) x VLC x 1000 (g/kg)	/BW ^{0.75}	x MW (ug/umol)/1000 (ug/mg)
umol/h/mg MP	umol/h/g liver	umol/h	umol/h/kg BW ^{0.75}	mg/h/kg BW ^{0.75}

In Vitro Value	x Scaling factor	x Tissue weight	/BW ^{0.75}	x MW = In vivo parameter (unit in PBPK model)
0.053	50.00	4791.89	198.01	17.53
	x MPPGL (mg MP/g liver)	x BW (kg) x VLC x 1000 (g/kg)	/BW ^{0.75}	x MW (ug/umol)/1000 (ug/mg)
umol/h/mg MP	umol/h/g liver	umol/h	umol/h/kg BW ^{0.75}	mg/h/kg BW ^{0.75}

Biological Scaling	VmaxLUC (mg/h/kg BW ^{0.75})	In Vitro Value
Female Mouse	Values	0.028
LUNG	Scaling & calculation	
	Unit	umol/h/mg MP

Biological Scaling	VmaxLUC (mg/h/kg BW ^{0.75})	In Vitro Value
Male Mouse	Values	0.14
LUNG	Scaling & calculation	
	Unit	umol/h/mg MP

Biological Scaling	KFLUC (L/h/kg BW ^{0.75})	In Vitro Value
Female Rat	Values	0.00073

LUNG	Scaling & calculation	
	Unit	L/h/mg MP

Biological Scaling	KFLUC (L/h/kg BW ^{0.75})	In Vitro Value
Male Rat	Values	0.00080
LUNG	Scaling & calculation	
	Unit	L/h/mg MP

Biological Scaling	KFLUC (L/h/kg BW)	In Vitro Value
Mixed gender Human	Values	1.49E-14
LUNG	Scaling & calculation	
	Unit	L/h/mg MP

Biological Scaling	VmaxLUC (mg/h/kg BW ^{0.75})	In Vitro Value
Male Mouse	Values	7.62E-05

Alternal Scaling

LUNG	Scaling & calculation	
	Unit	umol/h/mg MP

x Scaling factor	x Tissue weight	/BW ^{0.75}	x MW = In vivo parameter (unit in PBPK model)	Biological Scaling
23.00	0.165	2.03	0.18	Female Mouse
x MPPGLU (mg MP/g lung)	x BW (kg) X VLUC X 1000 (g/kg)	/BW ^{0.75}	x MW (ug/umol)/100 (ug/mg)	KIDNEY
umol/h/g lung	umol/h	umol/h/kg BW ^{0.75}	mg/h/kg BW ^{0.75}	

x Scaling factor	x Tissue weight	/BW ^{0.75}	x MW = In vivo parameter (unit in PBPK model)	Biological Scaling
23	0.918	10.27	0.91	Male Mouse
x MPPGLU (mg MP/g lung)	x BW (kg) X VLUC X 1000 (g/kg)	/BW ^{0.75}	x MW (ug/umol)/100 (ug/mg)	KIDNEY
umol/h/g lung	umol/h	umol/h/kg BW ^{0.75}	mg/h/kg BW ^{0.75}	

x Scaling factor	x Tissue weight			Biological Scaling
23	0.084			Female Rat

x MPPGLU (mg MP/g lung)	X VLUC X 1000 (g/kg)		
umol/h/g lung	L/h/fraction Lung		

KIDNEY

x Scaling factor	x Tissue weight		
23	0.092		
x MPPGLU (mg MP/g lung)	X VLUC X 1000 (g/kg)		
umol/h/g lung	L/h/fraction Lung		

Biological Scaling
Male Rat
KIDNEY

x Scaling factor	x Tissue weight		
23	2.60E-12		
x MPPGLU (mg MP/g lung)	X VLUC X 1000 (g/kg)		
L/h/g lung	L/h/fraction Lung		

Biological Scaling
Mixed gender Human
Kidney

x Scaling factor	x Tissue weight	/BW ^{0.75}	x MW = In vivo parameter (unit in PBPK model)
2.30E+01	9.32E-01	3.85E-02	3.41E-03

x MPPGLU (mg MP/g lung)	x BW (kg) X VLUC X 1000 (g/kg)	$/BW^{0.75}$	x MW (ug/umol)/100 (ug/mg)
umol/h/g lung	umol/h	umol/h/kg BW ^{0.75}	mg/h/kg BW ^{0.75}

KFKIC (L/h/kg BW ^{0.75})	In Vitro Value	x Scaling factor	x Tissue weight		
Values	0.0004184	11.0	0.07685		
Scaling & calculation		x MPPGK (mg MP/g kidney)	x BW (kg) x VKC x 1000 (g/kg)		
Unit	L/h/mg MP	L/hr/g kidney	L/hr/fraction kidney		

VmaxKIDc (mg/h/kg BW ^{0.75})	In vitro value (Yang et al. 2012, Table 3)	x Scaling factor	x Tissue weight	/BW ^{0.75}	x MW = In vivo parameter (unit in PBPK model)
Values	0.010	11.0	0.075	0.84	0.07
Scaling & calculation		x MPPGK (mg MP/g kidney)	x BW (kg) x VKC x 1000 (g/kg)	/BW ^{0.75}	x MW (ug/umol)/10 00 (ug/mg)
Unit	umol/h/mg MP	umol/h/g kidney	umol/h	umol/h/kg BW ^{0.75}	mg/h/kg BW ^{0.75}

VmaxKIDc (mg/h/kg BW ^{0.75})	In Vitro Value	x Scaling factor	x Tissue weight	/BW ^{0.75}	x MW = In vivo parameter (unit in PBPK model)
Values	0.00357	11.0	0.095	0.22	0.019

Scaling & calculation		x MPPGK (mg MP/g kidney)	x BW (kg) x VKC x 1000 (g/kg)	/BW ^{0.75}	x MW (ug/umol)/100 (ug/mg)
Unit	umol/h/mg MP	umol/h/g kidney	umol/h	umol/h/kg BW ^{0.75}	mg/h/kg BW ^{0.75}

VmaxKIDc (mg/h/kg BW ^{0.75})	In Vitro Value	x Scaling factor	x Tissue weight	/BW ^{0.75}	x MW = In vivo parameter (unit in PBPK model)
Values	0.00405	11.0	0.146	0.27	0.024
Scaling & calculation		x MPPGK (mg MP/g kidney)	x BW (kg) x VKC x 1000 (g/kg)	/BW ^{0.75}	x MW (ug/umol)/100 (ug/mg)
Unit	umol/h/mg MP	umol/h/g kidney	umol/h	umol/h/kg BW ^{0.75}	mg/h/kg BW ^{0.75}

in vitro metabolic constant not reported in Yang et al. 2012					

Uses IVIVE scaling approach from the Yoon report. (human

Cumulative (mg)
TSTOP 336 hrs
Exposure: 6 hr/day 5 days/week
Revised parameters from MCMC of In Vitro

Female Mouse InitialParms		
ppm	Amt. Metab.	Amt. Metab.
	Liver	Lung
12.8	1.22	1.20
32	3.11	1.91
80	7.90	2.52

Cumulative (mg)		
Human InitialParms		
ppm	Amt. Metab.	Amt. Metab.
	Liver	Lung
12.8	0.30	0.0078
32	0.74	0.0112
80	1.85	0.016

Cumulative (mg)		
Human Continuous Exposure (1 ppm)		
HumanParms Continuous Exposure		
PPM	Amt. Metab.	Amt. Metab.
	Liver	Lung
2.80E-04	3.56E-05	3.24E-06
1.00E-03	1.27E-04	1.16E-05
5.00E-03	6.37E-04	5.78E-05
1.00E-02	1.27E-03	1.15E-04
5.00E-02	6.37E-03	5.71E-04
1.00E-01	1.27E-02	1.13E-03
5.00E-01	6.38E-02	5.09E-03
1.00E+00	1.28E-01	9.09E-03
5.00E+00	6.42E-01	2.44E-02
1.00E+01	1.29E+00	3.09E-02
5.00E+01	6.45E+00	3.91E-02
1.00E+02	1.29E+01	4.05E-02

lung Vmax calculated using approach from methylene chloride - scaling liver in vitro vmax to lung based on ratio

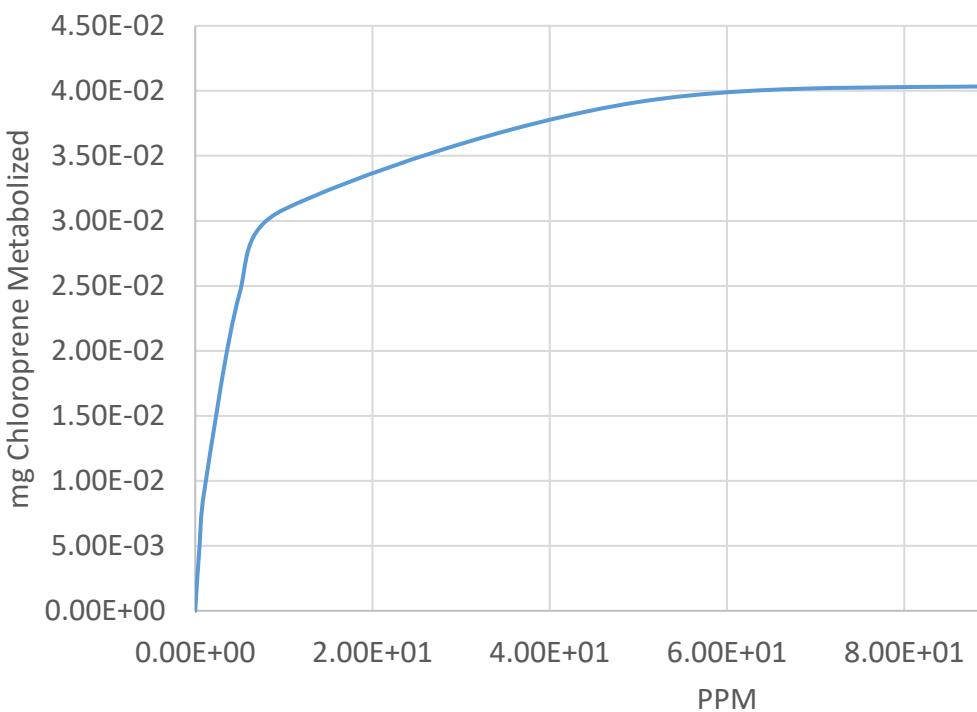
o data with flux included

Amt. Metab.
Kidney
0.040
0.10
0.26

Amt. Metab.
Kidney
-
-
-

Amt. Metab.
Kidney
-
-
-
-
-
-
-
-
-
-
-
-

Concentration Response Lung



io of ethoxycoumarin metabolism in lung to liver)

